

2-Isopropyl-6-methyl-4-pyrimidone
2814-20-2 | DTXSID1027502

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 6.94

Global applicability domain: Inside

Local applicability domain index: 6.93e-01

Confidence level: 4.19e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methylparaben</div> <div>Measured: 8.57</div> <div>Predicted: 7.06</div>	<div>Image not found</div> <div>1-Octanol</div> <div>Measured: 6.03</div> <div>Predicted: 5.95</div>	<div>Image not found</div> <div>Cyclohexanol</div> <div>Measured: 5.18</div> <div>Predicted: 4.72</div>
<div>Image not found</div> <div>1-Hexanol</div> <div>Measured: 5.18</div> <div>Predicted: 4.67</div>	<div>Image not found</div> <div>Dipropylamine</div> <div>Measured: 3.59</div> <div>Predicted: 4.37</div>	